PROTEIN CHARACTERIZATIONS BY CHIRAL VIBRATIONAL SUM FREQUENCY GENERATION SPECTROSCOPY

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Characterization of protein structures at interfaces in situ and in real time is important to solve fundamental and engineering problems. Nonetheless, such characterization remains challenging because it requires methods to be both selective to interfaces and protein structures. We show that chiral vibrational sum frequency generation spectroscopy (SFG) can provide peptide amide I and N-H stretching vibrational signals that are free of water background and characteristic to parallel beta-sheet, anti-parallel beta-sheet, alpha-helix, 3-10 helix, and disordered structures, thus enabling characterization of protein secondary structures at interfaces, similar to circular dichroism for characterizing protein structures in solution. Using chiral SFG, we monitor misfolding of an amyloid protein, measure interfacial protein orientation, derive new methods for probing backbone proton exchange, and examine two-dimensional crowding effects on protein folding. Moreover, we observe chiral SFG stretching modes of water molecules associated with a beta-sheet protein. This result reveals that achiral water molecules can be organized by the protein into chiral supermolecular structures. The result also implies that chiral SFG can be a promising vibrational probe for water structures in protein hydration. These recent developments demonstrate that chiral SFG can provide an array of new tools for addressing biological and biomedical problems related to protein structures.